

On quantum averaging, quantum KAM and quantum diffusion

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Dedicated to the memory of Mark Iosifovich Vishik.

Abstract

For nonautonomous Hamiltonian systems and their quantisations we discuss properties of the quantised systems, related to those of the corresponding classical systems, described by the KAM-related theories: the proper KAM, the averaging theory, the Nekhoroshev stability, and the diffusion.

1 Introduction

Consider a classical nonautonomous Hamiltonian system on the phase-space $T^*\mathbb{T}^d = \mathbb{R}^d \times \mathbb{T}^d = \{(p, q)\}$ or $T^*\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$ with a Hamiltonian $H(p, q, t)$:

$$\dot{p} = -\nabla_q H, \quad \dot{q} = \nabla_p H. \quad (1)$$

The corresponding quantum Hamiltonian operator is obtained by replacing in $H(p, q, t)$ the variable q_j , $j = 1, \dots, d$, by the operator which acts on complex functions $u(x)$ as multiplying by x_j , and replacing each p_j by the operator $\frac{\hbar}{i} \frac{\partial}{\partial x_j}$, where \hbar is the Planck constant.³ The Hamiltonian operator $\mathcal{H} = H(\frac{\hbar}{i} \nabla_x, x, t)$ defines a quantum system, and a classical problem of the quantum mechanics, streaming from its first years of existence, is to study (spectral) properties of the operator \mathcal{H} and the properties of the corresponding evolutionary equation

$$i\hbar \dot{u}(t, x) = \mathcal{H}u(t, x), \quad (2)$$

in their relation with the classical system (1).

For example, if

$$H(p, q, t) = |p|^2 + V(t, q), \quad (3)$$

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³This rule of quantisation is the most common, but certainly it is not unique. More generally one may replace q_j and p_j by any operators Q_j and P_j such that $[Q_j, P_k] = i\hbar \delta_{j,k}$, for all j and k .

then

$$\mathcal{H} = \mathcal{H}_t = -\hbar^2 \Delta + V(t, x), \quad (4)$$

i.e. \mathcal{H} is the Schrödinger operator with the potential V .

In this paper we discuss properties of the Hamiltonian operator \mathcal{H} , corresponding to properties of system (1), described by the KAM-related theories. Namely, by the proper KAM, the averaging, the Nekhoroshev stability, and the diffusion (this list by no means is canonical; it corresponds to the authors' taste). We discuss results for quantum systems (2) which we regard as parallel to the three classical theories above, mostly restricting ourselves to the case of periodic boundary conditions $x \in \mathbb{T}^d$ and assuming that $\hbar = \text{const}$. Scaling x and t in the dynamical equation (2), (4) we achieve $\hbar = 1$. A discussion concerning semiclassical limit $\hbar \rightarrow 0$, when it is not appropriate to scale \hbar to 1, is contained in Section 6. There we consider the equations in the whole space, $x \in \mathbb{R}^d$, since for the periodic boundary conditions the corresponding results are less developed.

All quantum results we discuss deal with non-autonomous equations (2), (4), so their classical analogies are “KAM-related” theories for non-autonomous Hamiltonian systems (3). We do not touch very interesting, important and complicated problem of constructing eigenfunctions of nearly integrable Hamiltonian operators by quantasing KAM-tori of the corresponding autonomous Hamiltonian systems (see [Laz93]).

Let $u(t)$ be a solution of the equation (2), (4). Multiplying the equation by \bar{u} and integrating over \mathbb{T}^d we get that $|u(t)|_{L_2}^2 = \text{const}$. Write $u(t, x) = \sum_s u_s(t) \varphi_s(x)$, where $\{\varphi_s\}$ are eigenfunctions of the “unperturbed” Hamiltonian operator. Then $\sum |u_s(t)|^2 \equiv \text{const}$. What happens to the quantities $|u_s(t)|^2$ as t grows, i.e. how the total probability $\sum |u_s(t)|^2$ is distributed between the states $s \in \mathbb{Z}^d$ when t is large? This is the question which is addressed by the theorems we discuss.

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2 Quantum averaging

2.1 Averaging and adiabatic invariance

Let a classical Hamiltonian (3) have the form

$$H(p, q, \varepsilon t) = H_\varepsilon = |p|^2 + V(\varepsilon t, q), \quad (5)$$

where the unperturbed Hamiltonian $|p|^2 + V(\tau, q)$, $\tau = \text{const}$, is integrable for each τ . Let $I_j, 1 \leq j \leq d$, be the corresponding actions. The classical averaging principle (e.g., see in [AKN06, LM88]) implies that each action is an adiabatic

invariant, namely if $u_\varepsilon(t)$ is a solution of the perturbed equation $(1)_{H=H_\varepsilon}$, then $I_j(u_\varepsilon(t))$ stays almost constant on time-intervals of order ε^{-1} . The averaging principle is a heuristic statement, and it does not always lead to correct results. The adiabatic invariance for classical systems is discussed in more details in Section 6.

Now consider the quantum system, corresponding to the Hamiltonian above:

$$\dot{u} = -i(-\Delta u + V(\varepsilon t, x)u), \quad x \in \mathbb{T}^d. \quad (6)$$

We assume that the function $V(\tau, x)$ is C^2 -smooth bounded and denote by A_t the linear operator in (6),

$$A_t = -\Delta + V(\varepsilon t, x).$$

Let $\{\varphi_s(\tau), s \in \mathbb{Z}^d\}$ and $\{\lambda_s(\tau)\}$ be the eigenvectors and the eigenvalues of A_τ , where each $\lambda_s(\tau)$ is continuous in τ . Let $u(t, x)$ be a solution of (6), equal at $t = 0$ to a pure state,

$$u(0, x) = \varphi_{s_0}(0), \quad (7)$$

such that for each εt , $\lambda_{s_0}(\varepsilon t)$ is an isolated eigenvalue of $A_{\varepsilon t}$ of a constant multiplicity. Consider expansion of $u(t, x)$ over the basis $\{\varphi_s(\tau), s \in \mathbb{Z}^d\}$:

$$u(t, x) = \sum_s u_s(t) \varphi_s(\varepsilon t).$$

The quantum adiabatic theorem says that $u(t, x)$ stays close to the eigenspace, corresponding to $\lambda_{s_0}(\varepsilon t)$:

Theorem 2.1. (*M. Born, V. Fock [BF28] and T. Kato [Kat50]*)

$$\sup_{0 \leq t \leq \varepsilon^{-1}} \sum_{s: \lambda_s(\varepsilon t) \neq \lambda_{s_0}(\varepsilon t)} |u_s(t)|^2 \rightarrow 0 \quad \text{as } \varepsilon \rightarrow 0. \quad (8)$$

This is a very general result which remains true for systems in the whole space (when $x \in \mathbb{R}^d$) if the operator $A_{\varepsilon t}$ has mixed spectrum, but $\lambda_{s_0}(\varepsilon t)$ always is an isolated eigenvalue of constant multiplicity, see in [LM88]. The case when this eigenvalues may be approached by other eigenvalues is considered in [AE99].

Both for classical and quantum systems, adiabatic theorems are considered often on infinite time interval $-\infty < t < \infty$ under condition that the dependence of the potential V on time disappears fast enough as $t \rightarrow \pm\infty$, and the system is sufficiently smooth. In this case, for classical Hamiltonians with $d = 1$, difference of values of actions on trajectory at $t \rightarrow \pm\infty$ tends to 0 much faster than ε as $\varepsilon \rightarrow 0$; in analytic case this difference is $O(\exp(-\text{const}/\varepsilon))$, see [LL60] and references in [AKN06], Sect. 6.4.5. For quantum systems, if for $\tau \rightarrow -\infty$ all the probability is concentrated in the states, corresponding to the eigenvalue $\lambda_{s_0}(\tau)$, then all the probability but a very small remnant will be absorbed by these states as $\tau \rightarrow +\infty$. In analytic case this remnant is $O(\exp(-\text{const}/\varepsilon))$ [Nen93, JP93] (this result also follows from the calculus, developed in [Sjo93]).

We will return to the quantum adiabaticity in Section 6. We note that also there are adiabatic theorems for systems where the Hamiltonian slowly depends not only on time, but also on a part of the space-variables, e.g. see [AKN06], Sect. 6.4.1 for classical systems and [BDT06] for quantum systems.

2.2 Around Nekhoroshev's Theorem.

Let us start with classical systems. Let $H_\varepsilon(p, q) = h_0(p) + \varepsilon h_1(p, q)$, where the function h_0 is analytic and steep (e.g., it is strictly convex, for the definition of steep functions see [Nek77] and [LM88, AKN06]). Let $(p(t), q(t))$ be a solution of (1). Then there are $a, b > 0$ such that

$$|p(t) - p(0)| \leq \varepsilon^a \quad \forall |t| \leq e^{\varepsilon^{-b}}, \quad (9)$$

see in [Nek77, LM88, AKN06]. There are many related results. For example: let

$$H_\varepsilon(p, q, t) = h_0(p) + \varepsilon h_1(\omega t; p, q), \quad \omega \in \mathbb{R}^N,$$

where h_1 is an analytic function on $\mathbb{T}^N \times \mathbb{R}^d \times \mathbb{T}^d$, $N \geq 1$. Then for a typical ω estimate (9) is true. In particular, let us take

$$H_\varepsilon(p, q, t) = |p|^2 + \varepsilon V(\omega t; q).$$

The corresponding quantised Hamiltonian is the operator $-\Delta + \varepsilon V(\omega t; x)$, and the evolutionary equation is

$$\dot{u} = -i(-\Delta u + \varepsilon V(\omega t; x)u). \quad (10)$$

Do we have for solutions of (10) an analogy of the Nekhoroshev estimate (9)? I.e. is it true that actions of the unperturbed system, evaluated along solutions of the perturbed equation (10), do not change much during exponentially long time? It turns out that a weaker form of this assertion holds true, even when $\varepsilon = 1$! Let us consider the equation

$$\dot{u} = -i(-\Delta u + V(t, x)u), \quad (11)$$

and consider the squared r -th Sobolev norm of u :

$$\|u\|_r^2 = \sum_{s \in \mathbb{Z}^d} |u_s|^2 (1 + |s|^2)^r, \quad r \in \mathbb{R}.$$

This is a linear combination of the actions for the unperturbed system with $V = 0$.

Theorem 2.2. ([Bou99a]). *Let $V(t, x) = \tilde{V}(\omega t, x)$, where $\omega \in \mathbb{R}^N$ is a Diophantine vector and \tilde{V} is a smooth function on $\mathbb{T}^N \times \mathbb{T}^d$. Then for each $r \geq 1$ there exists $c(r)$ such that any solution $u(t)$ of (11) satisfies*

$$\|u(t)\|_r \leq \text{Const} \cdot (\ln t)^{c(r)} \|u_0\|_r, \quad \forall t \geq 2. \quad (12)$$

So if u_0 is smooth, then the high states u_s stay almost non-excited for very long time. We miss a result which would imply that the quantity in (8), calculated for solutions of (11), (7) stays small for long time.

It is surprising that a weaker version of this result holds for potentials V which are not time-quasiperiodic:

Theorem 2.3. ([Bou99b]). *Let V be smooth and C^k -bounded uniformly in (t, x) for each k . Then for each $r \geq 1$ and $a > 0$ there exists C_a such that*

$$\|u(t)\|_r \leq C_a t^a \|u_0\|_s, \quad \forall t \geq 2.$$

Also see [Del10]. If the potential $V(t, x)$ is analytic, then the norm $\|u(t)\|_r$ satisfies (12), see [Wan08]. We are not aware of any classical analogy of these results.

3 Quantum KAM

Let $(p, q) \in \mathbb{R}^d \times \mathbb{T}^d$. Consider integrable Hamiltonian $h_0(p) = |p|^2$ and its time-quasiperiodic perturbation $H_\varepsilon(p, q) = h_0(p) + \varepsilon V(\omega t, q)$, $\omega \in \mathbb{R}^n$, where V is analytic. For the corresponding Hamiltonian equation we have a KAM result: *For a typical $(p(0), q(0))$ and a typical ω the solution $(p(t), q(t))$ is time-quasiperiodic.*

The quantised Hamiltonian defines the dynamical equation (10). We regard the vector ω as a parameter of the problem: $\omega \in U \subseteq \mathbb{R}^n$. We abbreviate $L^2 = L^2(\mathbb{T}^d, \mathbb{C})$ and provide this space with the exponential basis

$$\{e^{is \cdot x}, s \in \mathbb{Z}^d\}.$$

For any linear operator $B : L^2 \rightarrow L^2$ let $(B_{ab}, a, b \in \mathbb{Z}^d)$ be its matrix in this basis.

The theorem below may be regarded as a quantum analogy of the KAM theorem above. For $d = 1$ it is proven in [BG01], and for $n \geq 2$ – in [EK09]. We do not know how to pass in this result to the semiclassical limit.

Theorem 3.1. *If $\varepsilon \ll 1$, then for most ω we can find an φ -dependent complex-linear isomorphism $\Psi(\varphi) = \Psi_{\varepsilon, \omega}(\varphi)$, $\varphi \in \mathbb{T}^N$,*

$$\Psi(\varphi) : L^2 \rightarrow L^2, \quad u(x) \mapsto \Psi(\varphi)u(x),$$

and a bounded Hermitian operator $Q = Q_{\varepsilon, \omega}$ such that a curve $u(t) \in L^2$ solves eq. (10) if and only if $v(t) = \Psi(t\omega)u(t)$ satisfies

$$\dot{v} = i(\Delta v - \varepsilon Qv).$$

The matrix (Q_{ab}) is block-diagonal, i.e. $Q_{ab} = 0$ if $|a| \neq |b|$, and it satisfies

$$Q_{ab} = (2\pi)^{-n-d} \int \int V(\varphi, x) e^{i(a-b)} dx d\varphi + O(\varepsilon^\gamma), \quad \gamma > 0.$$

Moreover, for any $p \in \mathbb{N}$ we have $\|Q\|_{H^p, H^p} \leq C_1$ and $\|\Psi(\varphi) - \text{id}\|_{H^p, H^p} \leq \varepsilon C_2$.

Here “for most” means “for all $\omega \in U_\varepsilon \subset U$, where $\text{mes}(U \setminus U_\varepsilon) \leq \varepsilon^\kappa$ for some $\kappa > 0$ ”. In particular, for any ω as in the theorem all solutions of eq. (10) are almost-periodic functions of time. Their Sobolev norms are almost constant:

Corollary 3.2. *For ω as in the theorem and for any p solutions of (10) satisfy*

$$(1 - C\varepsilon)\|u(0)\|_p \leq \|u(t)\|_p \leq (1 + C\varepsilon)\|u(0)\|_p, \quad \forall t \geq 0.$$

This property is called the *dynamical localisation*.

Proof. Since Q is block-diagonal, then $\|v(t)\|_p = \text{const.}$ Since $v(t) = \Psi(t)u(t)$ and $\|\Psi - \text{id}\|_{H^p, H^p} \leq \varepsilon C_2$, then the estimate follows. \square

Remarks. 1) Let $n = 0$. Then (10) becomes the equation $\dot{u} = -i(\Delta u + \varepsilon V(x)u)$. Theorem states that this equation may be reduced to a block-diagonal equation $\dot{u} = -iAu$, where $A_{ab} = 0$ if $|a| \neq |b|$. This is a well known fact.

2) For $n = 1$ the theorem's assertion is the Floquet theorem for the time-periodic equation (10). In difference with the finite-dimensional case, this is a perturbative result, valid only for 'typical' frequencies $\omega \in \mathbb{R}$ and small ε .

Proof of the Theorem. Eq. (10) is a non-autonomous linear Hamiltonian system in L^2 :

$$\dot{u} = -i \frac{\delta}{\delta \bar{u}} H_\varepsilon(u), \quad H_\varepsilon(u) = \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle + \frac{1}{2} \varepsilon \langle V(\varphi_0 + t\omega, x)u, \bar{u} \rangle.$$

Consider the extended phase-space $L^2 \times \mathbb{T}^n \times \mathbb{R}^n = \{(u, \varphi, r)\}$. There the equation above can be written as the autonomous Hamiltonian system

$$\begin{aligned} \dot{u} &= -i \frac{\delta}{\delta \bar{u}} h_\varepsilon(u, \varphi, r), \\ \dot{\varphi} &= \nabla_r h_\varepsilon = \omega, \\ \dot{r} &= -\nabla_\varphi h_\varepsilon, \end{aligned}$$

where $h_\varepsilon(u, \varphi, r, \varepsilon) = \omega \cdot r + \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle + \frac{1}{2} \varepsilon \langle V(\varphi, x)u, \bar{u} \rangle$. So h_ε is a small perturbation of the integrable quadratic Hamiltonian $h_0 = \omega \cdot r + \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle$. To perturbations of h_0 applies the KAM-theorem from [EK10]. To show how this implies the Theorem 3.1 let us write h_ε as

$$h_\varepsilon(u, \varphi, r, \varepsilon) = \omega \cdot r + \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle + \varepsilon f(u, \varphi, r).$$

In our case $f = \frac{1}{2} \langle V(\varphi, x)u, \bar{u} \rangle$. The theorem below is the main result of [EK10].

Theorem 3.3. *There exist a domain $\mathcal{O} = \{\|u\| < \delta\} \times \mathbb{T}^n \times \{|r| < \delta\}$ and a symplectic transformation $\Phi : \mathcal{O} \rightarrow L^2 \times \mathbb{T}^n \times \mathbb{R}^n$ which transforms h_ε to*

$$h_0 = \omega' \cdot r + \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle + \varepsilon \langle Qu, \bar{u} \rangle + f'(u, \varphi, r),$$

where $f' = O(|u|^3) + O(|r|^2)$.

Torus $T_0 = 0 \times \mathbb{T}^n \times 0$ is invariant for the transformed system, so $\Phi(T_0)$ is invariant for the original equation. This is the usual KAM statement. Now it is trivial since it simply states that $u(t) \equiv 0$ is a solution on the original equation.

But the KAM theorem above tells more. Simple analysis of the proof (see a Remark in [EK2]) shows that if the perturbation εf is quadratic in u and r -independent, then the KAM-transformations are linear in u and do not change ω . So the transformed Hamiltonians stay quadratic in u . Hence, the Hamiltonian h_0 is such that $f' = 0$. That is,

$$h_0 = \omega' \cdot r + \frac{1}{2} \langle \nabla u, \nabla \bar{u} \rangle + \varepsilon \langle Qu, \bar{u} \rangle.$$

This proves Theorem 3.1.

4 Quantum diffusion.

Let $(p, q) \in R^d \times \mathbb{T}^d$. Consider $H_\varepsilon(p, q) = |p|^2 + \varepsilon V(\omega t, q)$, where $\omega \in \mathbb{R}^N$ and V is analytic. Then

- i) by KAM, for a typical ω and typical initial data (p_0, q_0) the solution such that $(p(0), q(0)) = (p_0, q_0)$ is time-quasiperiodic;
- ii) for exceptional ω and (p_0, q_0) we “should” have the Arnold diffusion: the action $p(t)$ of a corresponding solution slowly “diffuses away” from p_0 .

As before, the quantised Hamiltonian defines the dynamical equation (10).

Claim 4.1. Let $d = 1$, $N \geq 2$ and the potential V is nondegenerate in a suitable sense. Then there exist a smooth function $u(0, x)$ and $\omega \in \mathbb{R}^N$ such that

$$\limsup_{t \rightarrow \infty} \|u(t)\|_s = \infty \tag{13}$$

for some $s \geq 1$.

An *example* of a time-periodic potential V , satisfying (13), is given in [Bou99a]. It is conjectured by H. Eliasson that the validity of the Claim for a *typical* potential follows from the method of his work [Eli02]. Proof of this assertion is a work under preparation.

5 Perturbed harmonic and anharmonic oscillators.

In Sections 3, 4 we deal with the evolutionary Schrödinger equation under periodic boundary conditions. Some similar results are available for equations in the whole space with growing potentials:

- Consider Schrödinger equation in \mathbb{R}^1 :

$$\dot{u} = -i \left(-u_{xx} + (x^2 + \mu x^{2m})u + \varepsilon V(t\omega, x)u \right),$$

where $\mu > 0$, $m \in \mathbb{N}$, $m \geq 2$; $V(\varphi, x)$ is C^2 -smooth in φ, x and analytic in φ , bounded uniformly in φ, x . An analogy of Theorem 3.1 holds. See [Kuk93] (Section 2.5) for the needed KAM-theorem.

- Due to Bambusi-Graffi [BG01], the result holds for non-integer m . That is, for equations

$$\dot{u} = -i(-u_{xx} + Q(x)u + \varepsilon V(\varphi_0 + t\omega, x)u),$$

where $Q(x) \sim |x|^\alpha$, $\alpha > 2$ as $|x| \rightarrow \infty$. The potential V may grow to infinity as $|x| \rightarrow \infty$.

- Liu-Yuan [LY10] allow faster growth of $V(x)$ in x . Their result applies to prove an analogy of Theorem 3.1 for the *quantum Duffing oscillator*

$$\dot{u} = -i(-u_{xx} + x^4 u + \varepsilon x V(\varphi_0 + t\omega, x)u).$$

- Due to Grebert and Thomann [GT11], the assertion holds for the perturbed harmonic oscillator

$$\dot{u} = -i(-u_{xx} + x^2 u + \varepsilon V(\varphi_0 + t\omega, x)u).$$

What happens in higher dimensions, $d \geq 2$? – This is completely unknown.

6 Quantum adiabatic theorem in semiclassical limit

In this Section we consider the classical system on $T^*\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$ with a Hamiltonian

$$H(p, q, \tau) = |p|^2 + V(\tau, q), \quad \tau = \varepsilon t, \quad (14)$$

and the corresponding quantum system

$$i\hbar \dot{u} = -\hbar^2 \Delta u + V(\tau, x)u = \mathcal{H}_\tau u, \quad \tau = \varepsilon t, \quad (15)$$

(see (4)). We assume that for each τ the potential $V(\tau, x)$ grows to infinity with $|x|$, so the operator \mathcal{H}_τ has a discrete spectrum.

We fix small enough ε that allows to make some statements about the dynamics of the classical system, and then pass to the limit as $\hbar \rightarrow 0$. This limiting dynamics may be quite different from that in Section 2.1 when \hbar is fixed and $\varepsilon \rightarrow 0$, as it was demonstrated by M. Berry [Ber84] in the following striking example. Let $d = 1$ and potential V for $\tau = \text{const}$ has two (non-symmetric) potential wells. Generically, for $\tau = \text{const}$ and small enough \hbar each well supports a family of pure quantum states localised mainly in this well. Consider a solution $u(t, x)$ of equation (15) with an initial condition which is a pure quantum state from the left well. For however small ε there exists $\hbar_0 = \hbar_0(\varepsilon) > 0$ such that if $0 < \hbar < \hbar_0$, then for each $t \in [0, 1/\varepsilon]$ the function $u(t, \cdot)$ is localised in the same left well. On the other hand, under some rather general assumptions, for however small \hbar there exist $\varepsilon_0 = \varepsilon_0(\hbar)$ and positive constants $a_1 < a_2$, such that if $0 < \varepsilon < \varepsilon_0$ then the function $u(t, \cdot)$ is localised in the right well for $a_1 \hbar / \varepsilon \leq t \leq a_2 \hbar / \varepsilon$.

Discussion of the case $\varepsilon \sim \hbar$ is contained in [Kar90]. In what follows ε_0, c, c_i are positive constants.

6.1 Systems with one degree of freedom

Assume first that classical Hamiltonian (14) has one degree of freedom. We suppose that V is C^∞ -smooth and that in the phase plane of the Hamiltonian system (14) for each $\tau = \text{const}$ there is a domain filled by closed trajectories. In this domain we introduce action-angle variables $I = I(p, q, \tau)$, $\chi = \chi(p, q, \tau) \bmod 2\pi$ (i.e. $\chi \in \mathbb{T}^1$). Invert these relations: $p = p(I, \chi, \tau)$, $q = q(I, \chi, \tau)$. Suppose that there is an interval $[a_1, b_1]$, $0 < a_1 < b_1$, such that the map $I, \chi, \tau \mapsto p, q, \tau$ is smooth for $I \in [a_1, b_1]$, $\chi \in \mathbb{T}^1$, $\tau \in [0, 1]$. We express Hamiltonian (14) via the action variable and slow time: $H(p, q, \tau) = E(I, \tau)$.

For $\varepsilon > 0$ let $p(t), q(t)$ be a solution of the perturbed system with the Hamiltonian $H(p, q, \varepsilon t)$.

Theorem 6.1. (see, e.g., [Arn89]) *There exist ε_0, c_1 such that for $0 < \varepsilon < \varepsilon_0$ we have*

$$|I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| < c_1 \varepsilon \quad \text{for } 0 \leq t \leq 1/\varepsilon.$$

Now assume that for each $\tau = \text{const} \in [0, 1]$, and each $I_* \in (a_1, b_1)$ Hamiltonian H (14) has a unique trajectory with the action $I = I_*$. Consider the corresponding quantum system (15). The operator \mathcal{H}_τ has a series of eigenfunctions $\varphi_s(\tau) = \varphi_s(\tau, x)$ such that

$$\|\varphi_s(\tau)\| = 1, \quad \varphi_s(\tau, x) \rightarrow 0 \quad \text{as } x \rightarrow \infty, \quad (16)$$

and the corresponding eigenvalues are $\lambda_s(\tau) = E(I_s, \tau) + O(\hbar^2)$, where $I_s = \hbar(s + 1/2) \in [a_1, b_1]$ (this is the Bohr-Sommerfeld quantisation rule, see [MF81]). We assume that V is such that the convergence to zero in (16) is faster than $|x|$ in any negative power. Let $u(t, x)$ be a solution of non-stationary equation (15) with a pure state initial condition $u(0, x) = \varphi_{s_0}(0)$. Denote by $\mathbb{P}_{(\alpha, \beta)}(\tau)$ the orthogonal projector in $L^2(\mathbb{R})$ onto the linear span of vectors $\varphi_s(\tau)$ with $I_s \in (\alpha, \beta)$. The approach in [Bor78] leads to the following

Conjecture 6.2. There exist ε_0, c_1 such that if $0 < \varepsilon < \varepsilon_0$ and $0 < \hbar \leq \varepsilon$, then for any $m \geq 1$ and a suitable $c_2(m) > 0$ we have

$$\sup_{0 \leq t \leq \varepsilon^{-1}} \|u - \mathbb{P}_{(I_{s_0} - c_1 \varepsilon, I_{s_0} + c_1 \varepsilon)} u\| < c_2(m) \left(\frac{\hbar}{\varepsilon} \right)^m. \quad (17)$$

Thus $u(t, \cdot)$ stays close to the eigenspace that corresponds to eigenvalues from $O(\varepsilon)$ -neighbourhood of $E(I_{s_0}, \varepsilon t)$.

6.2 Systems with several degrees of freedom

Now let classical Hamiltonian (14) has $d > 1$ degrees of freedom. As before, we assume that $V \in C^\infty$. For each $\tau = \text{const}$ let the corresponding Hamiltonian system be completely integrable and in its phase space there is a domain filled by invariant tori. In this domain we introduce action-angle variables

$I = I(p, q, \tau)$, $\chi = \chi(p, q, \tau) \in \mathbb{T}^d$. Invert these relations: $p = p(I, \chi, \tau)$, $q = q(I, \chi, \tau)$. Suppose that there is a compact domain $\mathcal{A} \Subset \mathbb{R}_+^d$ such that the map $I, \chi, \tau \mapsto p, q, \tau$ is smooth for $I \in \mathcal{A}, \chi \in \mathbb{T}^d, \tau \in [0, 1]$. We express Hamiltonian (14) via the action variables and slow time, $H(p, q, \tau) = E(I, \tau)$, and denote by $\omega(I, \tau) = \partial E / \partial I$ the frequency vector of the unperturbed motion. We assume that the system is non-degenerate or iso-energetically nondegenerate (see definition in [Arn89], Appendix 8). The dynamics of the variables $(I, \chi)(t) = (I, \chi)(p(t), q(t), \varepsilon t)$ is described by a Hamiltonian of the form (see [Arn89], Sect. 52F)

$$\mathcal{H}(I, \chi, \tau, \varepsilon) = E(I, \tau) + \varepsilon H_1(I, \chi, \tau), \quad (18)$$

where H_1 is a smooth function on $\mathcal{A} \times \mathbb{T}^d \times [0, 1]$.

Let K_0 be a compact set in \mathbb{R}^{2d} . For $(p_0, q_0) \in K_0$ denote by $(p, q)(t) = (p, q)(t, p_0, q_0)$ a solution of the perturbed system with initial condition $(p, q)(0) = (p_0, q_0)$.

Theorem 6.3. (see, e.g., [AKN06, LM88]). *If $0 < \varepsilon < \varepsilon_0$, then*

$$\int_{K_0} \sup_{0 \leq t \leq \varepsilon^{-1}} |I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| dp_0 dq_0 < c_1 \sqrt{\varepsilon}.$$

In systems with $d > 1$ degrees of freedom the value of action-vector as a function of time may change considerably for some initial conditions due to the effect of resonance between unperturbed frequencies, i.e. components of the vector $\omega(I, \tau)$. We say that there is a resonance for some (I, τ) if $(k \cdot \omega)(I, \tau) = 0$ for a suitable vector $k \in \mathbb{Z}^d \setminus \{0\}$ (here \cdot denotes the Euclidian scalar product).

Now consider corresponding quantum system (15). Under some conditions, the operator \mathcal{H}_τ has a series of eigenfunctions $\varphi_s(\tau) = \varphi_s(\tau, x)$, $s \in \mathbb{Z}^d$, satisfying (16), with eigenvalues $\lambda_m(\tau) = E(I_m, \tau) + O(\hbar^2)$, where $I_m = \hbar(m + \frac{1}{4}\kappa) \in \mathcal{A}$, $m \in \mathbb{Z}_+^d$, and $\kappa \in \mathbb{Z}^d$ is the vector of the Maslov-Arnold indices [MF81] (the Bohr-Sommerfeld quantisation rule). Consider now the solution $u(t, x)$ of non-stationary equation (15) with a pure state initial condition $u(0, x) = \varphi_{m_0}(0)$. If we fix some small \hbar and proceed to the limit as $\varepsilon \rightarrow 0$, then Theorem 2.1 would apply. However, now we are interested in another limit, when a small ε is fixed and $\hbar \rightarrow 0$. Not much is known about the corresponding limiting dynamics. So we will formulate natural *hypotheses* about the limiting quantum dynamics as $\hbar \rightarrow 0$ and will use them jointly with the known results about dynamics for classical Hamiltonian (14) with small ε .

For Theorem 2.1 to hold it is important that $\lambda_{m_0}(\tau)$ is an isolated eigenvalue for all τ . Consider the distance between $\lambda_m(\tau)$ and $\lambda_{m_0}(\tau)$, where $m, m_0 \in \mathbb{Z}^d$ are such that $m \neq m_0$ and $|m - m_0| \sim 1$:

$$\begin{aligned} \lambda_m(\tau) - \lambda_{m_0}(\tau) &= E(I_m, \tau) - E(I_{m_0}, \tau) + O(\hbar^2) \\ &= (I_m - I_{m_0}) \cdot \omega(I_{m_0}, \tau) + O((I_m - I_{m_0})^2) + O(\hbar^2) \\ &= \hbar(m - m_0) \cdot \omega(I_{m_0}, \tau) + O(\hbar^2). \end{aligned}$$

Thus if there is no resonance at I_{m_0}, τ , then distance between $\lambda_{m_0}(\tau)$ and nearby eigenvalues is $\sim \hbar$. However, if there is a resonance $k \cdot \omega(I_{m_0}, \tau) = 0$, then $\lambda_{m_0+\nu k}(\tau) - \lambda_{m_0}(\tau) = O(\hbar^2)$ for integer $\nu \sim 1$. Thus classical resonances correspond to almost multiple points of the spectrum of the quantum problem. Therefore it seems that they should also manifest themselves in the quantum adiabaticity.

For Hamiltonian (14) there is a rather detailed information about dynamics in the two-frequency case $d = 2$. We will now use this information and the Bohr-Sommerfeld quantisation rule to state some conjectures about dynamics for the 2d quantum system (15).

Following P. Dirac [Dir25] we assume that ⁴

$$\omega_2 \frac{\partial \omega_1}{\partial \tau} - \omega_1 \frac{\partial \omega_2}{\partial \tau} - \left(\omega_2 \frac{\partial \omega_1}{\partial I} - \omega_1 \frac{\partial \omega_2}{\partial I} \right) \frac{\partial H_1}{\partial \chi} > c^{-1} \quad (19)$$

for all I, φ . General result by V. I. Arnold about averaging in two-frequency systems [Arn65, AKN06] implies that in this case

$$|I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| < c_1 \sqrt{\varepsilon} \quad \text{for } 0 \leq t \leq 1/\varepsilon. \quad (20)$$

On the basis of the Bohr-Sommerfeld quantisation rule and by analogy with Conjecture 6.2 it is natural to conjecture that for $0 \leq t \leq 1/\varepsilon$ the total probability $|u(t)|_{L_2}^2$ is mostly concentrated in the states, corresponding to actions from the $C\sqrt{\varepsilon}$ -vicinity of the original action I_{s_0} .

Now assume that instead of (19) the following condition is satisfied (cf. the forth footnote)

$$\omega_2 \frac{\partial \omega_1}{\partial \tau} - \omega_1 \frac{\partial \omega_2}{\partial \tau} > c^{-1}. \quad (21)$$

This is a particular case of a condition introduced by V. I. Arnold in [Arn65]. If, in addition to (21), some general position condition is satisfied (see details in [AKN06]), then estimate (20) in which $\sqrt{\varepsilon}$ is replaced with $\sqrt{\varepsilon} |\ln \varepsilon|$ holds for all initial data outside a set of measure $O(\sqrt{\varepsilon})$ [AKN06], Sect. 6.1.8. The later set mainly consists of initial data for trajectories with *capture into resonance*, along these trajectories actions change by values ~ 1 . Since for some initial data $I(0), \chi(0)$ the solution $I(t)$ is not localised in the vicinity of $I(0)$, then we should not expect for the quantum system (15) any estimate similar to that of Conjecture 6.2, where the amplitudes of eigenmodes tend to 0 as $\hbar \rightarrow 0$ outside some small interval of actions.

Consider classical Hamiltonian (14) under condition (21). Then the capture is only possible for a finite number of resonances, and the dynamics with a capture into resonance $k_1 \omega_1 + k_2 \omega_2 = 0$ with co-prime k_1, k_2 is the following

⁴Condition (19) just means that the ratio of frequencies changes with non-zero rate along solutions of the system with Hamiltonian (18): $\omega_2^2 \frac{d}{dt} \left(\frac{\omega_1}{\omega_2} \right) > c^{-1} \varepsilon$. Similarly, condition (21) means that ratio of frequencies changes with non-zero rate in adiabatic dynamics: $\omega_2^2 \frac{d}{dt} \left(\frac{\omega_1}{\omega_2} \right)_{I=\text{const}} > c^{-1} \varepsilon$.

[Nei05]. Denote $(I, \chi)(t) = (I, \chi)(p(t), q(t), \varepsilon t)$. Suppose that at the initial moment $t = 0$ we have no resonance:

$$k_1\omega_1(I(0), 0) + k_2\omega_2(I(0), 0) \neq 0,$$

and let $\tau_* \in (0, 1)$ be the first moment when the resonance occurs:

$$k_1\omega_1(I(0), \tau_*) + k_2\omega_2(I(0), \tau_*) = 0.$$

Then for $0 \leq \varepsilon t \leq \tau_*$ the values of actions are approximately conserved:

$$I(t) = I(0) + O(\sqrt{\varepsilon} \ln \varepsilon).$$

For $\tau_* \leq \varepsilon t \leq 1$ the system is captured into resonance, and evolution of actions is described by two relations:

$$\begin{aligned} k_1\omega_1(I(t), \varepsilon t) + k_2\omega_2(I(t), \varepsilon t) &= O(\sqrt{\varepsilon} \ln \varepsilon), \\ k_2I_1(t) - k_1I_2(t) &= k_2I_1(0) - k_1I_2(0) + O(\sqrt{\varepsilon} \ln \varepsilon). \end{aligned}$$

First of them means that the system stays near the resonance, while the second says that the dynamics has an approximate first integral. Jointly the two relations approximately define the trajectory $I(t)$ for $\tau_* \leq \varepsilon t \leq 1$.

Based on this description and the Bohr-Sommerfeld quantisation rule, by analogy with Conjecture 6.2 we conjecture that for the quantum problem (15) the capture in resonance in the classical system (14) results in transfer of an $C\varepsilon$ -amount of the total probability from the vicinity of the initially excited pure state, corresponding to the action I_{s_0} , to the vicinity of a state $s_t \in \mathbb{Z}^2$ such that the lattice vector $I(t) = \hbar(s_t + \frac{1}{4}\kappa)$ satisfies the two relations above. This transfer happens for $t \geq \varepsilon^{-1}\tau_*$. When $\hbar \rightarrow 0$, this $C\varepsilon$ -amount stays positive of order ε .

For the dynamics of captured into resonances phase points also there is a more detailed description [Nei05]. Consider the resonant phase $\gamma = k_1\chi_1 + k_2\chi_2$. It turns out that the behaviour of γ is described by an auxiliary Hamiltonian system with one degree of freedom and the Hamiltonian of the form

$$F = \sqrt{\varepsilon} (\alpha(\tau)p_\gamma^2/2 + f(\gamma, \tau) + L(\tau)\gamma).$$

Here p_γ, γ are canonically conjugate variables, function f is 2π -periodic in γ , and $\alpha, L \neq 0$. In the phase portrait of the system for frozen τ there are domains of oscillations of γ . Motion in these domains can be approximately represented as composition of motion along a trajectory of Hamiltonian F with frozen τ and slow evolution of this trajectory due to the change of τ . This evolution follows the adiabatic rule: the area surrounded by the trajectory remains constant. In the original variables p, q this motion is represented as a motion along slowly evolving torus. Angular variables on this torus are γ and $\psi = l_1\varphi_1 + l_2\varphi_2$, where l_1 and l_2 are integers such that $k_1l_2 - k_2l_1 = 1$. This torus drifts along the resonant surface $k_1\omega_1 + k_2\omega_2 = 0$ as it was described above. It is not known which quantum object corresponds to it.

References

- [AE99] J. Avron and J. Elgert, *Adiabatic theorem without gap conditions*, Commun. Math. Phys. **203** (1999), 445–463.
- [AKN06] V. I. Arnold, V.V. Kozlov, and A. I. Neishtadt, *Mathematical aspects of classical and celestial mechanics*, 3rd ed., Springer-Verlag, Berlin, 2006.
- [Arn65] V.I. Arnold, *Conditions for the applicability, and estimate of the error, of an averaging method for systems which pass through states of resonance in the course of their evolution*, Sov. Math., Dokl. **6** (1965), 331–334.
- [Arn89] V. I. Arnold, *Mathematical methods in classical mechanics*, 3rd ed., Springer-Verlag, Berlin, 1989.
- [BDT06] V. Belov, S. Dobrokhotov, and T. Tudorovskiy, *Operator separation of variables for adiabatic problems in quantum and wave mechanics*, J. Engineering Math. **55** (2006), 183–237.
- [Ber84] M.V. Berry, *The adiabatic limit and the semiclassical limit*, J.Phys. A: Math., Gen. **17** (1984), 1225–1233.
- [BF28] M. Born and V. Fock, *Beweis des adiabaten satzes*, Z. Phys. **51** (1928), 165–180.
- [BG01] D. Bambusi and S. Graffi, *Time quasi-periodic unbounded perturbations of Schrödinger operators and KAM methods*, Comm. Math. Physics **219** (2001), 465–480.
- [Bor78] V. A. Borovikov, *Fields in slowly irregular waveguides and a variation of adiabatic invariant problem (in Russian)*, Preprint 99 of Keldysh Applied Mathematics Institute (1978), 1–66.
- [Bou99a] J. Bourgain, *Growth of Sobolev norms in linear Schrödinger equations with quasi-periodic potentials*, Comm. Math. Phys. **204** (1999), 207–247.
- [Bou99b] ———, *On growth of Sobolev norms in linear Schrödinger equation with smooth time-dependent potentials*, J. Anal. Math. **77** (1999), 315–348.
- [Del10] J-M Delort, *Growth of Sobolev norms of solutions of linear Schrödinger equations on some compact manifolds*, Int. Math. Res. Note **2010** (2010), 2305–2328.
- [Dir25] P. A. M. Dirac, *The adiabatic invariance of the quantum integrals*, Proc. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci. **107** (1925), 725–734.

- [EK09] H. L. Eliasson and S. B. Kuksin, *On reducibility of Schrödinger equations with quasiperiodic in time potentials*, Comm. Math. Phys. **286** (2009), 125–135.
- [EK10] ———, *KAM for the non-linear Schrödinger equation*, Annals of Mathematics **172** (2010), 371–435.
- [Eli02] H. L. Eliasson, *Ergodic skew-systems on $T^d \times SO(3, R)$* , Ergod.Th. Dynam. Sys **22** (2002), 1429–1449.
- [GT11] B. Grébert and L. Tomann, *KAM for the quantum harmonic oscillator*, Comm. Math. Phys. **307** (2011), 383–427.
- [JP93] A. Joye and C.E. Pfister, *Superadiabatic evolution and adiabatic transition probability between two nondegenerate levels isolated in the spectrum*, J. Math. Phys. **34** (1993), 454–479.
- [Kar90] M. V. Karasev, *New global asymptotics and anomalies for the problem of quantization of the adiabatic invariant*, Functional Analysis and Its Applications **24** (1990), no. 2, 104–114.
- [Kat50] T. Kato, *On the adiabatic theorem of quantum mechanics*, J. Phys. Soc. J. Jpn. **5** (1950), 435–439.
- [Kuk93] S. B. Kuksin, *Nearly integrable infinite-dimensional Hamiltonian systems*, Springer-Verlag, Berlin, 1993.
- [Laz93] V. F. Lazutkin, *KAM theory and semiclassical approximations to eigenfunctions*, Springer, Berlin, 1993.
- [LL60] L.D. Landau and E.M. Lifshitz, *Course of theoretical physics. vol. 1: Mechanics*, Addison-Wesley, Reading MA, 1960.
- [LM88] P. Lochak and C. Meunier, *Multiphase averaging for classical systems*, Springer-Verlag, New York–Berlin–Heidelberg, 1988.
- [LY10] J. Liu and X. Yuan, *Spectrum for quantum Duffing oscillator and small-divisor equation with large-variable coefficient*, Comm. Pure Appl. Math **63** (2010), 1145–1172.
- [MF81] V.P. Maslov and M.V. Fedoryuk, *Semiclassical approximation in quantum mechanics*, Reidel, Boston, 1981.
- [Nei05] A.I. Neishtadt, *Capture into resonance and scattering on resonances in two-frequency systems*, Proc. Steklov Inst. Math. **250** (2005), 183–203.
- [Nek77] N. N. Nekhoroshev, *Exponential estimate of the stability of near integrable Hamiltonian systems*, Russ. Math. Surveys **32** (1977), no. 6, 1–65.

- [Nen93] G. Nenciu, *Linear adiabatic theory, exponential estimates*, Commun. Math. Phys. **152** (1993), 479–496.
- [Sjo93] J. Sjostrand, *Projecteurs adiabatiques du point de vue pseudodifférentiel*, C. R. Acad. Sci. **317** (1993), 217–220.
- [Wan08] W.-M. Wang, *Logarithmic bounds on Sobolev norms for time dependent linear Schrödinger equations*, Comm. Partial Differential Equations **33** (2008), 2164–2179.